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HYDRODYNAMIC STUDY OF SMALL-SCALE UASB REACTOR BY COMPUTATIONAL FLUID DYNAMICS (CFD): SIMULATION AND VALIDATION

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ABSTRACT

A small-scale UASB reactor was modeled in order to evaluate its hydrodynamic behavior and compare CFD simulations with experimental results obtained on a laboratory scale. Simulations using Ansys® CFX™ were carried out with two different flow rates: A) 26.68 and B) 4.0 l d^{-1}. The reactor volume was 1.5 liters, with a useful volume of 1.38 liters. In addition to the CFD simulations, hydrodynamic tests with tracer injection were performed, both experimentally and in simulations. Residence time distribution (RTD) curves were obtained and the number of tanks-in-series (NTIS) model was used for determination of hydrodynamic behavior. The NTIS values calculated using CFD simulations were 5.55 and 4.76, for flow rates A and B, respectively. For the experimental analysis, the NTIS values were 6.67 and 5.54, for A and B flow rates, respectively. The Mann-Whitney U test was performed to confirm the similarity between CFD simulations and experimental tests. The results of the Mann-Whitney U test showed no statistically significant differences between the CFD simulations and experimental data. It can be concluded that CFD simulations are valid and can be used to analyze the hydrodynamic behavior of UASB reactors.

KEYWORDS: CFD, experimental, simulation, tracer injection tests

ESTUDO HIDRODINÂMICO DE REATOR UASB DE PEQUENA ESCALA POR DINÂMICA DE FLUIDO COMPUTACIONAL (CFD): SIMULAÇÃO E VALIDAÇÃO

RESUMO

Um reator UASB em pequena escala foi modelado para avaliar seu comportamento hidrodinâmico e comparar simulações de CFD com resultados experimentais obtidos em escala de laboratório. Foram realizadas simulações usando o Ansys® CFXTM com duas taxas de fluxo diferentes: A) 26,68 e B) 4,0 l d^{-1}. O volume do reator era de 1,5 litros, com um volume útil de 1,38 litros. Além das simulações de CFD, foram realizados testes hidrodinâmicos com injeção de traçador, tanto experimentalmente quanto nas simulações. Foram obtidas curvas de distribuição do tempo de residência (RTD) e o modelo de número de tanques em série (NTIS) foi usado para determinação do comportamento hidrodinâmico. Os valores de NTIS calculados usando simulações de CFD foram 5,55 e 4,76, para as taxas de fluxo A e B, respectivamente. Para a análise experimental, os valores de NTIS foram 6,67 e 5,54, para as taxas de fluxo A e B, respectivamente. O teste U de Mann-Whitney foi realizado para confirmar a similaridade entre as simulações de CFD e os testes experimentais. Os resultados do teste U de Mann-Whitney não mostraram diferenças estatisticamente significativas entre as simulações de CFD e os dados experimentais. Pode-se concluir que as simulações de CFD são válidas e podem ser usadas para analisar o comportamento hidrodinâmico dos reatores UASB.

Palavras chave: CFD, experimental, simulação, testes de injeção de traçador.

1 INTRODUCTION

Upflow anaerobic sludge blankets (UASB) are biological reactors that are used widely in wastewater treatment, especially in hot climates (Chernicharo et al., 2015). This technology can be used to treat both industrial and domestic wastewater and provides: (i) lower maintenance and operating costs when compared to aerobic systems; (ii) ready formation of dense granules and their maintenance at the inferior part of the reactor due to the reactor's hydrodynamics (Bhatti et al., 2014; Rodríguez-Gómez et al., 2014; Chernicharo et al., 2015); (iii) effective removal of organic matter coupled to biogas production (Hinken et al., 2014; Lu et al., 2015); and (iv) a low growth rate of the biomass, decreasing the frequency of the biomass discharges (Daud et al., 2018).

UASB performance, in terms of organic matter removal and energy yield, is usually run by two main interrelated factors: microbiological and hydrodynamic (Ren et al., 2009). Regarding the reactor hydrodynamics, it is known that this may be influenced by the mixing characteristics, presence of dead zones, short circuiting, and fluid velocities, which are usually not considered in most of the models applied for anaerobic digestion. Simulation in computational fluid dynamics (CFD) (Passos et al., 2014; Cruz et al., 2016) and laboratory experimental tests (stimulus-response techniques with tracers and related models) (Fia et al., 2016) are suitable methods to evaluate the reactor hydrodynamics. Moreover, CFD has an additional advantage as it can be used to a large extent to replace time-consuming and expensive experiments (Pourtousi et al., 2015).

In this context, systematic comprehension of the hydrodynamic behavior of a UASB, based on complete understanding of the flow patterns and their relation with the reactor performance, is still lacking. The resident time distribution (RTD) may be a useful tool to achieve this goal. The RTD can effectively describe the real hydraulic behavior and detect anomalies in biological reactors. Determination of the RTD is relatively simple and Levenspiel (1999) presents one of the best-known theoretical references on this subject. Previous studies on UASB hydrodynamics have shown that they could be well described by the number of tanks-in-series model (NTIS) (Fia et al., 2016).

The current study aimed to fully comprehend the hydrodynamic behavior of a small-scale UASB reactor through CFD simulation and real experimental tests. The tests were run by considering two different flow rates and the final method was validated by statistical analysis.

2 METHODOLOGY

2.1 Experimental apparatus

The small-scale UASB was made of acrylic and contained some MBBR (moving bed biofilm reactor) plastics to simulate the sludge blanket (Figure 1). Tap water was applied as the influent by a dosing pump (Grundfos, DDA). The reactor has a 2.0 cm buffer zone immediately above the entrance. Table 1 contains information regarding the reactor's structure.

Table 1: UASB characteristics.

Parameter/Unit	Value
Height (cm)	66
Larger diameter (cm)	10
Smaller diameter (cm)	5
Volume (L)	1.50
Effective volume (L)	1.38
Porosity (-)	0.88
Wall roughness (mm)	0.005

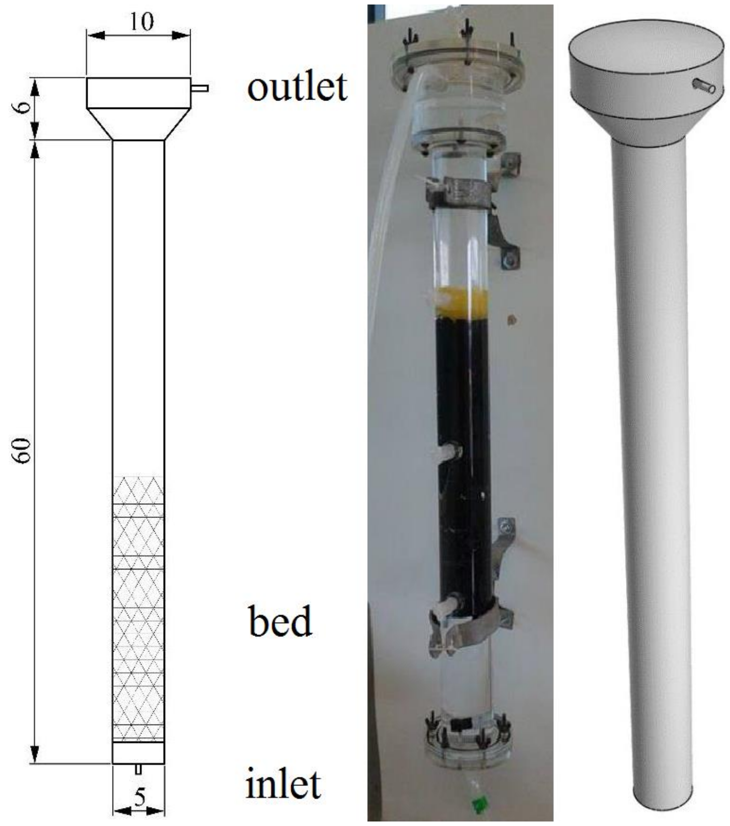


Figure 1: Schematic, real, and virtual perspective view of the small-scale UASB reactor.

2.2 Experimental procedure

The experimental work was performed by considering two different flow rates: 26.68 (C1) and 4.0 l d^{-1} (C2). The time taken for a fluid element to pass through a reactor, from its entry to its exit, is named the hydraulic retention time (HRT). The fluid movement can roam through various routes, remaining for different times within the reactor. In this study, the theoretical HRTs for each tested condition were 1h21min and 9h00min, respectively. These HRTs were calculated by considering the total reactor volume.

Based on the detection of the time that each fluid element spends passing through the reactor, the residence time distribution curve (RTD) was reached by injecting an input stream of 5.0 mL of sodium chloride (NaCl) at a concentration of 3.0 g l^{-1}(tracer).

This type of injection is called a “pulse injection” and its primal characteristic is that a small volume of tracer is needed to perform the experiment, compared to the full reactor volume. The tracer concentration (C) was continuously measured at the reactor outlet, along with the time, and resulted in a C curve, as expressed by Equation 1. The tracer concentration was indirectly assessed by the electrical conductivity monitoring (Vernier) and then converted to mg l^{-1} of tracer.

$$C_{pulse} = \int_0^{\infty} C.dt \qquad (1)$$

where C is the tracer concentration (mg l^{-1}) and t is the experiment time (min).

The average HRT was estimated by the data acquired during the experimental tests (Equation 2):

$$\overline{HRT} = \frac{\int_0^{\infty} t.C.dt}{\int_0^{\infty} C.dt} \qquad (2)$$

For the pulse injection, the RTD function, denominated the E curve, is defined by Equation 3:

$$E(t) = \frac{C(t)}{\int_0^{\infty} C(t).dt} \qquad (3)$$

where:

$$\int_0^{\infty} E(t).dt = 1 \qquad (4)$$

Prior to the NTIS model application and its integrated analysis with the kinect models, the function E_Θ (dimensionless concentration) was calculated (Equations 5 and 6), where $\mathbf{\Theta}$ is defined as the dimensionless time:

$$E_{\Theta} = \overline{HRT}.E \qquad (5)$$

$$\Theta = \frac{t}{\overline{HRT}} \qquad (6)$$

The number of tanks-in-series was calculated using Equation 7:

$$NTIS = \frac{1}{\sigma_{\Theta}^2} \qquad (7)$$

where σ_{Θ}^2 is the variance of the dimensionless residence time distribution, given in Equation (8):

$$\sigma_{\Theta}^2 = \frac{\sigma^2}{\overline{HRT}^2} \qquad (8)$$

The NTIS value is an important criterion for judging the flow patterns in a reactor. Commonly, NTIS = 1 represents a completely mixed flow system, however NTIS = ∞ indicates a plug-flow unit. The integration of a dynamic mass balance around the strand of reactors generates the RTD of the system. The dimensionless concentration of a tracer in the NTIS is given by Equation (9) (Levenspiel, 1999):

$$E_{\Theta} = NTIS.\frac{(NTIS.\Theta)^{NTIS-1}}{(NTIS-1)!}.e^{-NTIS.\Theta} \quad (9)$$

2.3 CFD Modelling Approach

The process of CFD modeling involves several essential steps: (i) build a three-dimensional geometry of the reactor (Figure 1); (ii) develop a mesh using finite elements or finite volumes; (iii) perform a grid independence test to choose the optimal mesh; (iv) define boundary conditions, calculation methods, and additional equations, and, finally, (v) process the results. In this study the CFD software used was Ansys 14.0®. The software package includes a geometry maker (DesingModeler^{TM}), a mesher (Meshing^{TM}), and pre-processing, processing, and post-processing modules (CFX^{TM}).

The simulation domain was represented by a geometric representation, so only the volume occupied by the fluid in the reactor was considered. In CFD simulations, the fluid volume in the reactor is divided into a mesh, which is comprised of a portion of "smaller" volumes, for which the mass conservation and momentum calculations are performed. In general, the finer the grid resolution, the more precise the results are expected to be (Li, Yang and Dai, 2009).

Therefore, two grids were constructed to choose the best one (M1 and M2), in terms of quality results and simulation processing time. The difference between the two meshes is in the refinement of the blanket region. The first mesh (M1) was constructed using a standard configuration of the software Meshing^{TM} and the second mesh (M2) relates to the refining performed only in the blanket. The CFD simulation should seek independence from the outcomes in relation to the density of the mesh adopted (Curi et al., 2017).

A series of tests are needed to ensure the mesh refinement and also to compare the results if the refinement does not change the results. All tests were performed with the same physical and boundary conditions. The primary endpoint of the level of mesh refinement is the simulation convergence.

CFD software usually contains tools that allow monitoring of convergence parameters. For example, CFX-Solver^{TM} allows the user to visualize the convergence degree of various parameters, such as the conservation of mass and momentum through RMS P-Mass, RMS U-Mom, RMS V-Mom, and RMS W-Mom criteria.

Other important parameters are RMS and RMS TurbKE K-O-TurbFreq, related to the model of turbulence k-ω shear stress transport (SST), and the Imbalance parameter. However, additional parameters can be used in the grid independence test, such as comparing the simulation results, for example, in this investigation, the reactor RTD curve for each level of mesh refinement.

The fundamental equations used in CFD simulations, such as conservation of mass, momentum, and energy, which are the basis of the CFD model, are available in several textbooks (e.g., Fortuna 2000). Besides these fundamental equations, another was added to the model to simulate the tracer test (Equation 10) as a result of a virtual tracer pulse injection in the first timestep (1s).

$$Tracer = \boldsymbol{step}((t-1[s])/1[s]) * \boldsymbol{step}((\gamma[s]-t)/1[s]) * \beta\ [kg\ s^{-1}] \tag{10}$$

where γ is the injection duration (seconds), and β is the load of tracer injected (kg s^{-1}) in the reactor.

The meshes analyzed in this study were exclusively comprised of unstructured tetrahedrals and volumes. Mesh independence was evaluated in two manners:

- observation of the Imbalance parameter (%) for the P-mass, U-Mom, V-Mom, W-Mom, and tracer variables, the latter variable was introduced by the authors. Note: the simulation was considered as acceptable when the Imbalance was below 1%;
- statistical analysis of the RTD curve simulation at each level of mesh refinement.

For the entire computational domain, water properties were defined at 30ºC (specific mass = 995.6 kgm^{-3}; molar mass = 18.02 $gmol^{-1}$; dynamic viscosity = 0.798 x 10^{-3} $N.sm^{-2}$; thermal conductivity = 0.6069 $Wm^{-1}K^{-1}$; specific heat capacity = 4172.7 $Jkg^{-1}K^{-1}$). The UASB blanket, as previously mentioned, was replicated with MBBR plastics, resulting in a porosity of 0.88. To simulate this porous medium, it was set up in CFX-Pre, a two-phase flow in the region of the blanket with the same porosity value.

Boundary conditions for the CFD simulations were like the experimental tests, due to the need to simulate the real conditions. All simulations were run under transient conditions. A Root Mean Square Error (RMS) of 10^{-5} was defined as the convergence criterion for all variables. Moreover, the total time simulation was chosen as a criterion for completion for two tested conditions.

Data regarding boundary conditions and transient simulations are displayed in Table 2.

Table 2: Boundary conditions and transient analysis for the CFD simulations (C1 and C2)

Parameter	**C1**	**C2**
	Value	
Flow rate (l.d^{-1})	26.68	4.0
Inlet velocity (m.s^{-1})	1.38 x 10^{-2}	2.37 x 10^{-3}
Outlet relative pressure (Pa)	0	0
Wall roughness (mm)	0.005	0.005
Porosity (-)	0.88	0.88
Total time simulation (min)	501	1995
Timestep (min)	3	15

The turbulence model was the SST (hybrid model of k-ε and k-ω) at 1%.

2.4 Validation Method

To analyze the similarity of the experimental data and the CFD simulations and further validate the model we compared:

- the number of NTIS;

- statistical analysis of RTD curves by applying (i) the Student's t test for samples that follow a standard distribution; (ii) the Mann-Whitney U test for samples that do not follow a normal distribution (nonparametric test for two independent samples); both tests considering a 5% significance level.

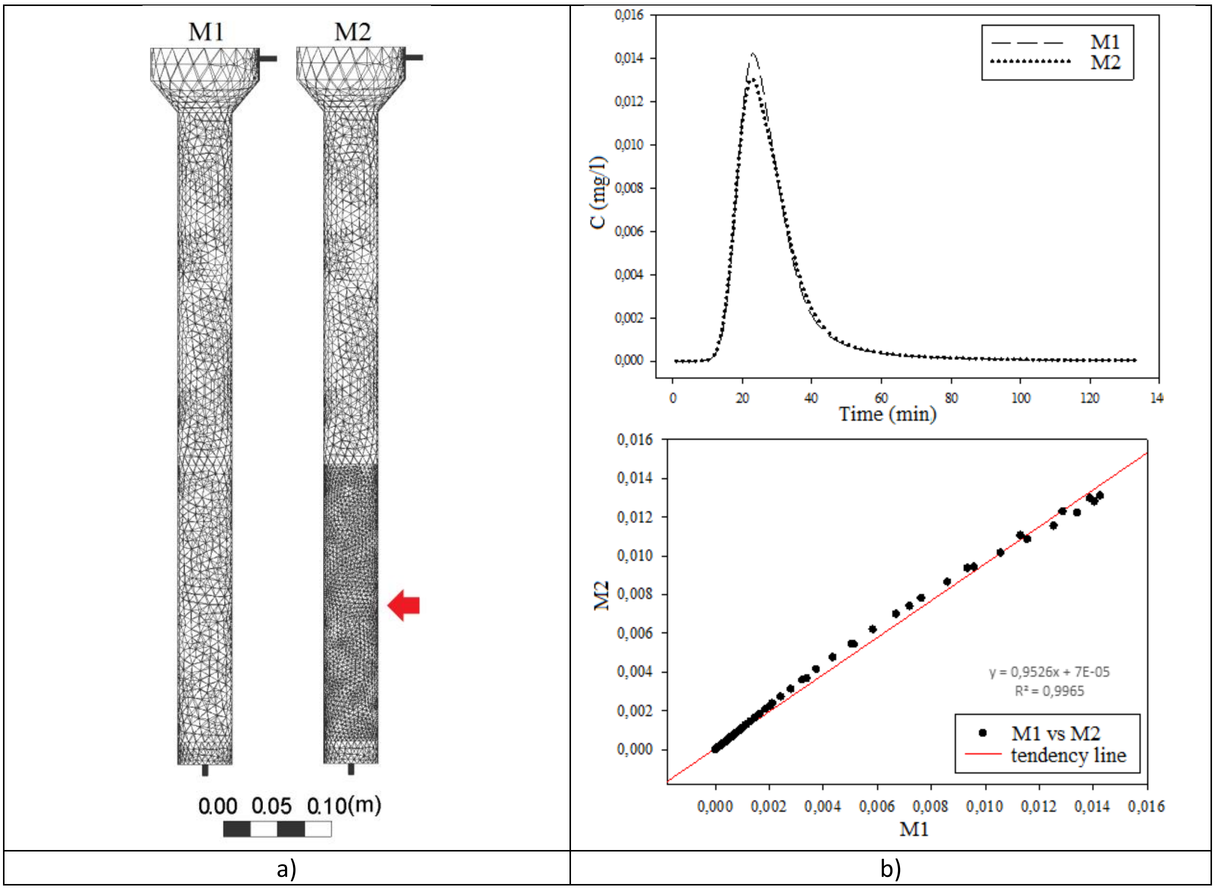
3 RESULTS AND DISCUSSION

3.1 Grid independence test

Figure 2a depicts the two meshes (M1 and M2) developed in this study (arrow indicates the area of refinement).

Meshes 1 and 2 were composed of nodes (junctions between tetrahedral elements) and elements (tetrahedral control volumes). M1 has 9307 nodes and 44505 elements, while M2 has 17100 nodes and 84023 elements. The Imbalance parameter reached values below 1% for all variables, indicating stability in the simulations.

To complete the grid independence test, the Mann-Whitney U test was applied to the RTD curves generated from the M1 and M2 simulations. The U test revealed that the difference in median values between the two curves was not large enough to rule out the possibility of random sampling variability. Therefore, there is no statistically significant difference (significance level of 5%, p-value of 0.804). Figure 2b presents the two curves interposed and the linear regression between the M1 and M2 RTD curves ($R^2 = 0.9965$).



a)

b)

Figure 2: a) Meshes 1 (standard) and 2 (refined). b) RTD curves of M1 and M2 and the linear regression between M1 and M2.

From these findings it can be concluded that both curves were statistically equal. Consequently, the mesh used in the CFD validation was M1, due to its lower computational requirement.

The test was performed with the input data relating to the C1 condition. Once a test has been conducted for one condition, its output can be leveraged for other conditions, i.e., the test was valid for conditions C1 and C2.

3.2 Hydrodinamic Analysis – Simulation and Experimentation

The CFD simulation for conditions C1 and C2 were carried out according to Table *2*. The velocity vectors and RTD curves (relating to the experimental, simulated, and NTIS model data) are illustrated in Figures 3 and 4.

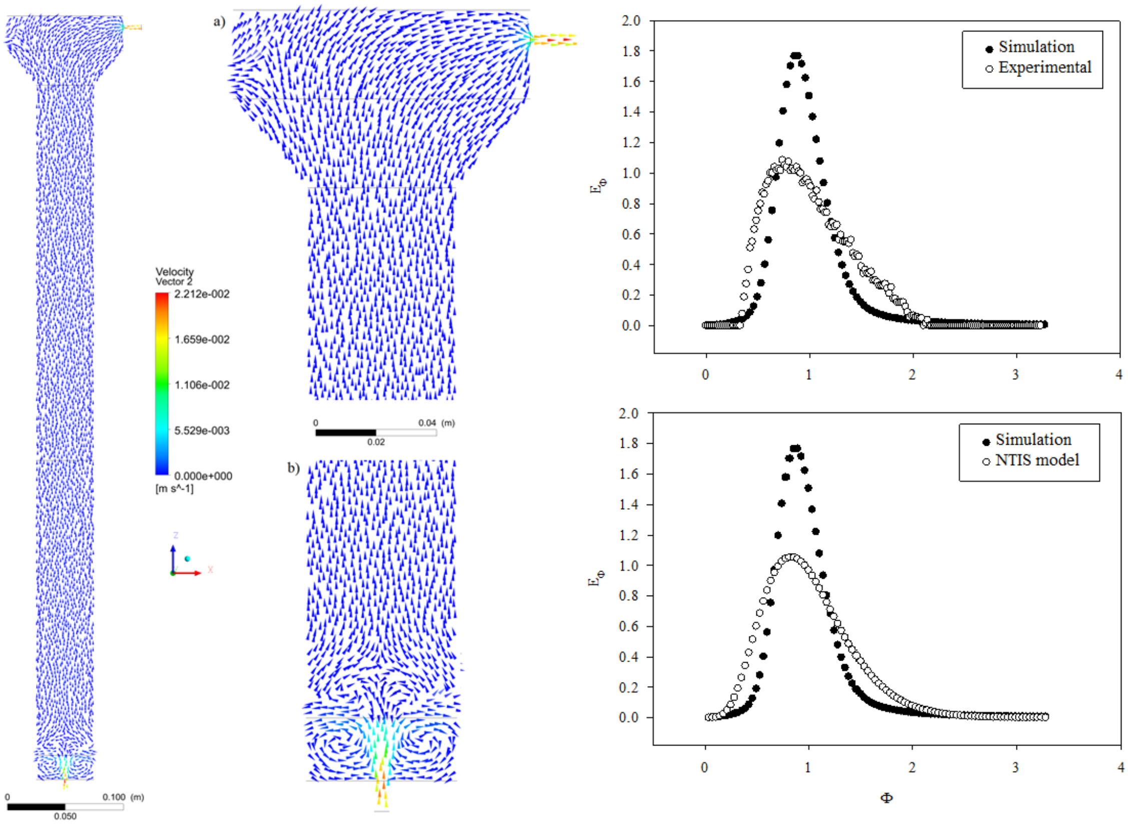


Figure 3 - Velocity vectors and RTD curves (simulated, experimental, and NITS model) for condition C1.

A uniform distribution of velocity vectors in the vertical direction and some recirculation zones can be observed in Figures 4 and 5. The buffer had a major influence on the even distribution of the flow (Figure 1), and plug-flow behavior is observed to the reactor's outlet.

The same comments can be made for condition C2, but it is important to mention that due to the low input flow, the C2 flow is also less turbulent than C1.

The hydrodynamic behavior and NTIS model results for conditions C1 and C2 are shown in Table 3.

Initially, it was observed that the NTIS values (experimental and simulated) were very close for both conditions (Table 3). This is borne out due to the boundary conditions and development of the three-dimensional model approach that is as close as possible to reality.

Table 3 – Hydrodynamic analysis for conditions C1 and C2.

Parameter	C1		C2	
	Simulation	Experimental	Simulation	Experimental
Theoretical HRT (h)	1.52	1.52	9.0	9.0
Average HRT (h)	1.40	2.57	9.8	9.4
σ_Θ^2 (-)	0.18	0.15	0.21	0.22
NTIS (-)	5.55	6.67	4.76	5.54

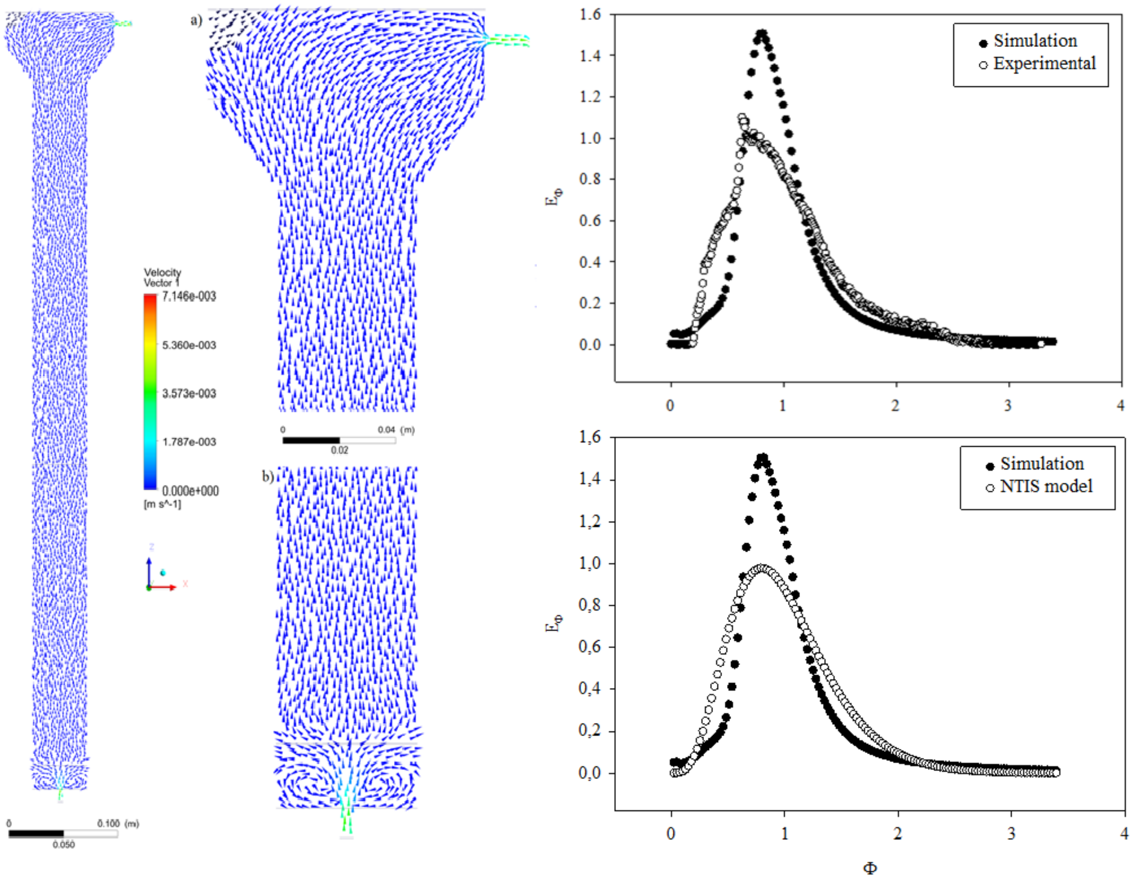


Figure 4 - Velocity vectors and RTD curves (simulated, experimental, and NITS model) for condition C2.

3.3 Model Validation

The validation was performed using statistical analysis. The Mann-Whitney U test was used because the experimental and simulated data do not follow normal distribution. The p-values for conditions C1 and C2 were 0.561 and 0.940, respectively, where ($\alpha = 0.05$). No significant statistical differences were identified for the conditions, as the p-values was less than the alpha. Thus, CFD simulations can be used to analyze the hydrodynamic behavior and the tracer test proposed by Levenspiel (1999).

This fact may contribute to new insights for bioreactor applications in engineering processes, as diverse configurations can be tested before constructing a real model, whether in small or full scale.

4 CONCLUSION

CFD was proven to be a powerful and innovative tool in the analysis of hydrodynamic behavior of a UASB system. It was possible to establish a higher level of confidence of this tool by experimental validation of the data obtained computationally.

As a result, it can be stated that the use of CFD software, such as CFX^{TM}, is essential in the development of reactors (of any kind) and in the understanding of their hydrodynamic behavior.

Through computer simulations, results that require long lead times and large financial resources can be reduced to the need for a computer, a software license, and a small amount of time.

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